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ABSTRACT

Presented are the teacher's guide and student materials for one of a series of self-instructional, computer-based learning modules for an introductory, undergraduate chemistry course. The student manual for this unit on Le Chatelier's principle includes objectives, prerequisites, pretest, instructions for executing the computer program, and problems. Included in the teacher's guide are implementation instructions, software, a sample run of the computer program in BASIC, and a listing of the computer program in BASIC. (BT)

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ED182120

CHEMICAL EQUILIBRIUM

UNIT 2. LE CHATELIER'S PRINCIPLE

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LOYOLA UNIVERSITY

A COMPUTER-ENRICHED MODULE
FOR INTRODUCTORY CHEMISTRY

U S DEPARTMENT OF HEALTH,
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SE 029 753

OBJECTIVES

When you finish this unit you will be able to

1. determine how a gaseous system in chemical equilibrium will react when one of several stresses is applied to it
   a. increasing or decreasing pressure (decreasing or increasing the volume)
   b. adding a reactant or a product of the reaction
   c. changing the temperature.
2. determine how a solution reaction at equilibrium will adjust when a stress is applied
   a. a reactant is added
   b. a product is added.
3. determine what happens to an equilibrium state of a chemical reaction involving a solid when more solid is added.

PREREQUISITES

Before you start this unit you should

1. know that the equilibrium state of any chemical system is characterized by the equilibrium constant.
2. know which concentrations are included in the equilibrium constant expression.

PRE-TEST

Write the expression for the equilibrium constant for each of the following systems:

1. $PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g)$
2. $PCl_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)$
3. $CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$
4. $CO(aq) + H_2O \rightleftharpoons CO_2(aq) + H_2(aq)$ (in aqueous solution)

Answers to the pre-test:

1. $K = \frac{[PCl_5]}{[PCl_3][Cl_2]}$
2. $K = \frac{[Cl_2][PCl_3]}{[PCl_5]}$
3. $K = [CO_2]$
4. $K = \frac{[CO_2][H_2]}{[CO]}$

INTRODUCTION

What happens when we disturb an equilibrium state? First, let us consider some everyday examples:

a. Suppose you add a large weight to the high end of a see-saw. What happens to the see-saw with the weight on it?

b. When you suddenly shift your weight in a rocking chair, what happens to the system (that is, you and the rocking chair)?

c. When you squeeze the middle of an inflated balloon, how does it respond?

It's clear that the answers are: (a) the upper end of the see-saw is now heavier and settles down to a new equilibrium situation, (b) you and the rocking chair shift to a new equilibrium position, and (c) the middle of the balloon is reduced in size while the ends enlarge in adjusting to a new equilibrium state.

All of the above cases have something in common, that is, when a stress is applied to an equilibrium system, the system adjusts by relieving the stress to reach a new equilibrium situation. The cases discussed above are summarized in the following table:

CASE	ORIGINAL EQUILIBRIUM STATE	STRESS	NEW EQUILIBRIUM STATE
a.	see-saw with the heavy end on the ground	weight applied to the light end	opposite end is now heavier -- and on the ground (stress is relieved)
b.	rocking chair with person in it	person moves	a new geometry of chair and person is reached (stress is relieved)
c.	inflated balloon	middle is squeezed	middle of the balloon is reduced while ends are enlarged

It is important to note that the imposed stress causes the system to react to relieve the stress. This generalization is often given the name "Le Chatelier's Principle".

The previous examples were obvious physical cases. What about chemical systems? Does something similar happen?

d. Suppose you have a beaker containing a saturated solution of NaCl (ordinary table salt) in water, with excess solid NaCl on the bottom of the beaker. Now stir in more distilled water. What happens to the system?

e. Suppose you open a bottle of soda pop. Before you opened it, the pressure of the gas above the solution was well above atmospheric pressure. After opening the bottle the pressure suddenly drops. What happens then?

In case (d), solid NaCl goes into solution while in case (e), CO_2 escapes as bubbles from the solution when the system is disturbed. In these cases, just as in physical systems in general, when a system in equilibrium is disturbed, the system reacts to relieve the stress or disturbance, thereby reaching a new equilibrium state.

In all of the previous examples, whether physical or chemical, we have seen how a system, when disturbed from equilibrium, reacts to the disturbance in such a way as to relieve the applied stress as it approaches a new equilibrium condition. Now let's try to see what happens in a chemical reaction when we disturb it. A way to

get some feeling for this type of system is to do the following computer exercise.

COMPUTER EXERCISE

Run the program LECHAT which simulates the behavior of a chemical system. You will be allowed to change the concentrations of any reactant or product as well as increase or decrease the pressure. Fill in the accompanying table (Do [A], [B], [C] increase or decrease?):

APPLIED STRESS	How Does the System React? [A]	[B]	[C]
ADD A			
ADD B			
ADD C			
INCREASE PRESSURE			
DECREASE PRESSURE			

Count the A, B, C molecules just as the stress is applied and after equilibrium is re-established. Does this reaction follow Le Chatelier's Principle? [ ]

Another reaction: Phosphorus trichloride reacts with chlorine to give phosphorus pentachloride:

$$PCl_3 + Cl_2 \rightleftharpoons PCl_5 \qquad \text{(all are gases)}$$

At a temperature of 250°C, one equilibrium condition is $[PCl_3] = 0.1$ moles/liter, $[Cl_2] = 0.1$ moles/liter, $[PCl_5] = 0.24$ moles/liter. Let us consider what will happen if we disturb the system in various ways:

a. Increase the pressure. A way to increase the pressure is to decrease the volume of the container. Suppose we squeeze the gas mixture into a volume which is one-half of its original volume. If the system does not react to this change then all the concentrations would double and would no longer satisfy the equilibrium condition. One way to alleviate the stress is for the system to subsequently react in a way to decrease the total pressure if there is some way, that is, by decreasing the total number of moles of gas in the container. A means to do this in this example is for PCl_3 molecules to combine with Cl_2 molecules to form PCl_5 molecules. Two molecules reacting to form one molecule diminishes the total number of molecules in the system. The important point is that the pressure will be modified only if there is some means which will allow it. In this reaction:

$$PCl_3 + Cl_2 \rightleftharpoons PCl_5$$

a reduction in pressure can occur if <u>one</u> PCl_5 molecule forms from <u>two</u> reactant molecules. Whenever a chemical reaction has a different number of gaseous molecules on the two sides of the equation then the effect of increasing pressure can be alleviated by the reaction proceeding to <u>decrease</u> the total number of molecules.

In other reactions, for instance,

$$H_2(g) + I_2(g) \rightleftharpoons 2\ HI(g)$$

reaction in either direction results in the same number of molecules. Hence, there is no effect of pressure on the relative equilibrium concentrations in this case.

b. Decrease the pressure. Conversely, decreasing the pressure (by increasing the volume and hence decreasing the total concentration) will disturb the system. It can adjust in a way to increase the pressure somewhat. The way to do this is for the chemical reaction to proceed in such a way as to create more molecules -- that is, by molecules of PCl_5 disappearing and two molecules (PCl_3 and Cl_2) taking the place of each lost PCl_5.

c. Add PCl_5. If we add PCl_5 to an equilibrium system, then the system will try to use up some of the added PCl_5 and a new equilibrium is established. Similarly, if we add PCl_3 or if we add Cl_2, the system will react to the disturbance in such a manner as to decrease the concentration of added molecules, that is, using up PCl_3 and Cl_2 molecules to produce PCl_5 molecules.

d. Increase the temperature. If we increase the temperature we add heat to the system. Suppose we had a reaction in which heat is given off:

$$A + B \rightleftharpoons C + \text{heat}\ .$$

How will this equilibrium system react if we increase its temperature? The system reacts just as Le Chatelier's Principle predicts: the system can act to relieve the stress by formation of more reactants A and B.

Problem 1. In each of the following reactions all components are gases. If the pressure is suddenly increased, what would have to happen in order for equilibrium to be re-established? (Would more reactants or products form?)

a) $2\ N_2O_5 \rightleftharpoons 4\ NO + O_2$

b) $SO_2Cl_2 \rightleftharpoons SO_2 + Cl_2$

c) $2\ NO_2Cl \rightleftharpoons 2\ NO_2 + Cl_2$

d) $N_2O_4 \rightleftharpoons 2\ NO_2$

e) $4\ NH_3 + 3\ O_2 \rightleftharpoons 2\ N_2 + 6\ H_2O$

f) $H_2 + I_2 \rightleftharpoons 2\ HI$

g) $2\ O_3 \rightleftharpoons 3\ O_2$

h) $CH_4 + Cl_2 \rightleftharpoons CH_3Cl + HCl$

Problem 2. In each of the following reactions all components are gases. If heat is added to the system (that is, if the temperature is raised), how will the system react to re-establish equilibrium?

a) $N_2 + 3\ H_2 \rightleftharpoons 2\ NH_3 + \text{heat}$

b) $2\ SO_2 + O_2 \rightleftharpoons 2\ SO_3 + \text{heat}$

c) $N_2 + O_2 + \text{heat} \rightleftharpoons 2\ NO$

A MOLECULAR UNDERSTANDING OF THE BEHAVIOR OF EQUILIBRIUM SYSTEMS

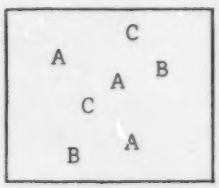
In a box full of gas, molecules are traveling rapidly, bouncing off walls and colliding with each other. For the reaction

$$PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g)$$

PCl_3 molecules collide with each other, with Cl_2 and with PCl_5. Sometimes when PCl_3 and Cl_2 molecules collide, a PCl_5 molecule can form. If we introduce more PCl_3 molecules into a gas already at equilibrium, there will suddenly be many more collisions of PCl_3 and Cl_2 molecules in a given time so more PCl_5 molecules will be able to form if this type of disturbance is made. Likewise with introducing more Cl_2. More collisions of Cl_2 and PCl_3 will occur so more PCl_5 can form. On the other hand, if we introduce PCl_5 into the gas at equilibrium, then there will suddenly be more PCl_5 molecules. So there will be more of them to break up -- and more reactant molecules will be formed as this happens.

Finally, what happens to the number of collisions of various types in a specific time if the concentrations of all species are suddenly increased? The same number of PCl_5 molecules undergo more collisions -- simply because the molecules are closer together. As a consequence, when the concentrations in this reaction are increased by decreasing the volume (or increasing the pressure) the result will be a tendency for more PCl_5 to form.

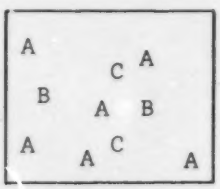
Initial State



A = PCl_3
B = Cl_2
C = PCl_5

IMMEDIATELY AFTER STRESS AT EQUILIBRIUM

PCl_3 added →



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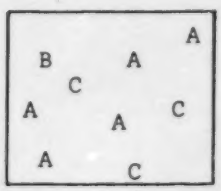
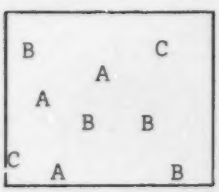


Cl_2 added →



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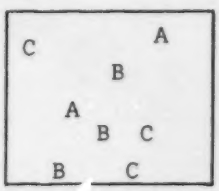
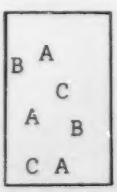


Pressure doubled →



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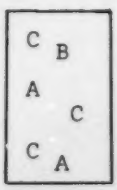

A REACTION IN SOLUTION

It makes no difference whether the reaction takes place in the gas phase or in solution. The effect of a disturbance on a system at equilibrium is quite similar. As an example, let's consider the reaction

$$CH_3COOC_2H_5 + H_2O \rightleftharpoons CH_3COOH + C_2H_5OH$$

ethyl acetate — acetic acid — ethyl alcohol

This reaction is the "hydrolysis" of ethyl acetate, a volatile solvent used in nail polish removers. It reacts with water to form acetic acid (found in vinegar) and ethyl alcohol (found in liquor). If we add ethyl acetate or water to this system at equilibrium we instantaneously add a large amount of reactant. Quite predictably the system responds to this stress by subsequent formation of the products. On the other hand, if we could find nothing better to do with ethyl alcohol and added it to the reaction mixture, the system would respond by subsequent formation of reactants.

Let's write down the expression for the equilibrium constant:

$$K = \frac{[CH_3COOH][C_2H_5OH]}{[CH_3COOC_2H_5]} .$$

The reaction takes place in aqueous solution and we are restricting our discussion to solutions in which H_2O is in very large excess. Hence $[H_2O]$ remains essentially constant and is included in the equilibrium constant. Of course, even though $[H_2O]$ does not appear in the equilibrium expression, addition of water, the solvent, does affect the reaction indirectly exactly as we would expect. If we added water to this reaction mixture at equilibrium we would suddenly decrease the concentrations of all the species in solution (except water, of course). Dilution of a solution has the same effect as increasing the volume does in a gas-phase equilibrium system. Subsequently more molecules would have to form in order for equilibrium to be re-established. Would the equilibrium be shifted by addition of solvent if the equilibrium constant were of the form $K = \frac{[A][B]}{[C][D]}$?

Problem 3. What reaction would occur after instantaneous addition of each reactant and product in the following reactions in dilute aqueous solution (in which H_2O is in very large excess)?

a) $C_4H_9Br(aq) + H_2O \rightleftharpoons C_4H_9OH(aq) + HBr(aq)$

tertiary butyl bromide — tertiary butyl alcohol

b) $Br_2(aq) + CH_3COCH_3(aq) \rightleftharpoons BrCH_2COCH_3(aq) + HBr(aq)$

acetone

REACTIONS INVOLVING PURE SOLIDS AND PURE LIQUIDS

Consider the following systems:

$$2\ NO(g) + Br_2(l) \rightleftharpoons 2\ NOBr(g)$$

$$CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$$

(The latter is a well-known industrial process for making lime from limestone, calcium carbonate, by heating.) In both of these systems the concentrations of the gases are independent of the amount of pure solid or pure liquid in which they are in equilibrium, so long as some solid or liquid is present. Write the expression for the equilibrium constants for these reactions.

Problem 4. What would happen in the example of heating $CaCO_3$ if we disturbed the equilibrium system by

a) adding more $CaCO_3$?

b) adding more CaO?

c) expanding the volume of the container?

Problem 5. What would happen in the case of $2\ NO(g) + Br_2(l) \rightleftharpoons 2\ NOBr(g)$ if we disturbed the equilibrium system by

a) adding NOBr(g)?

b) adding $Br_2(l)$?

c) expanding the volume of the container?

Problem 6. Write the expression for the equilibrium constant for each of the following reactions:

a) $FeO(s) + H_2(g) \rightleftharpoons Fe(s) + H_2O(g)$

b) $CO_2(g) + Zn(s) \rightleftharpoons CO(g) + ZnO(s)$

c) $Fe_2O_3(s) + 3\ H_2(g) \rightleftharpoons 2\ Fe(s) + 3\ H_2O(g)$

The CM Project

The Computer-enriched Module (CM) project is a collaborative effort by 19 faculty members in the disciplines of chemistry, mathematics and physics, to produce self-instructional computer-based materials at the introductory college level in those disciplines. Each module is designed to be usable in an academic environment with minimal computational facilities, and by students and faculty who are not programming experts. It may be used as an adjunct to standard textual materials, or in many cases, as a replacement for them. The primary aim of each module is to use the computer in such a way that students may take a more active role in the development and discovery of concepts and phenomena.

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TEACHER'S GUIDE TO

A MODULE ON CHEMICAL EQUILIBRIUM

UNIT 2. LE CHATELIER'S PRINCIPLE

A. KEITH JAMESON

LOYOLA UNIVERSITY

a computer-enriched module

for introductory chemistry

featuring the program

LECHAT

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TEACHER'S GUIDE TO UNIT ON LE CHATELIER'S PRINCIPLE OF THE CHEMICAL EQUILIBRIUM MODULE

EDUCATIONAL OBJECTIVES

The objective is to enable the student to qualitatively understand the effects of concentration on an equilibrium system.

The computer augmentation involves LECHAT, which simulates the effects of added reagents or changes in size of the container by a two-dimensional graphics display of a box with reactant and product molecules A, B, and C scattered in a random fashion throughout the box.

IMPLEMENTATION

In this unit some simple familiar physical systems are introduced with the hope that the student can see the plausibility of the generalization usually called Le Chatelier's Principle:

> "When a stress is applied to a system in equilibrium the system adjusts by relieving the stress to reach a new equilibrium state."

Two slightly more complicated systems (a. the two-phase solid NaCl and aqueous solution, and b. bottle of soda pop) are introduced to see that the general statement applies when the "stresses" are less familiar (adding a reagent and pressure change).

After this introduction the program LECHAT is run by the student. The gas phase reaction

$$A = B + C$$

is simulated. A container or "box" is printed out by the terminal with reactant and product molecules randomly distributed. When A, B, or C is added the system reacts to relieve the stress. The student can count the A, B, and C molecules just after the stress is added and after equilibrium is attained once more.

NOTE: The better student may realize that:

1. the stoichiometry of the reaction is obeyed

   $2A_i + B_i + C_i = 2A_f + B_f + C_f$

   (A_i, B_i, C_i are initial concentrations; A_f, B_f, C_f are final concentrations), and
2. the mass action expression is equal to the equilibrium constant <u>whenever</u> equilibrium has been attained.

After running LECHAT all students should see that adding reactant or product (or changing the pressure) produces a stress which the system <u>can</u> relieve.

The total time the student will spend on this unit is probably about one hour including about 15 minutes running LECHAT.

This unit should be used <u>before</u> standard textual material is assigned to the student. LECHAT is an abstraction of an experiment in which the student can choose how concentrations can affect an equilibrium system. It is an attempt to develop physical intuition. Consequently, the most likely uses for this unit are

1. as an adjunct to lectures on chemical equilibrium (coming <u>before</u> lectures on the effect of concentration).
2. as a unit for a self-paced course.

PROBLEM SOLUTIONS

1. In each of the following reactions all components are gases. If the pressure is suddenly increased what would happen in order for equilibrium to be re-established?

a.	$2N_2O_5 = 4NO + O_2$	reactant $[N_2O_5]$ increases
b.	$SO_2Cl_2 = SO_2 + Cl_2$	reactant $[SO_2Cl_2]$ increases
c.	$2NO_2Cl = 2NO_2 + Cl_2$	reactant increases
d.	$N_2O_4 = 2NO_2$	reactant increases
e.	$4NH_3 + 3O_2 = 2N_2 + 6H_2O$	reactant increases
f.	$H_2 + I_2 = 2HI$	no change
g.	$2O_3 = 3O_2$	reactant increases
h.	$CH_4 + Cl_2 = CH_3Cl + HCl$	no change

2. In each of the following reactions all components are gases. If heat is added to the system (that is, if the temperature is raised), how will the system react to re-establish equilibrium?

a.	$N_2 + 3H_2 = 2NH_3 + \text{heat}$	more reactants will form
b.	$2\ SO_2 + O_2 = 2SO_3 + \text{heat}$	more reactants will form
c.	$N_2 + O_2 + \text{heat} = 2NO$	more products will form

3. What reaction would occur after instantaneous addition of each reactant and product in the following reactions in dilute aqueous solution (in which H_2O is in very large excess)?

a. $C_4H_9Br + H_2O = C_4H_9OH + HBr$

addition of:

C_4H_9Br	more products form
water	more products form
C_4H_9OH	more reactants form
HBr	more reactants form

b. $Br_2 + CH_3COCH_3 = BrCH_2COCH_3 + HBr$

addition of:

Br_2 or CH_3COCH_3	more products form
HBr or $BrCH_2COCH_3$	more reactants form

4. What would happen in the example of heating $CaCO_3$ if we disturbed the equilibrium system by

   a. adding more $CaCO_3$? -- nothing (since it is a solid and has unit activity in equilibrium with the gas phase).
   b. adding more CaO? -- nothing (again a solid).
   c. expanding the volume of the container? -- again the finally established equilibrium condition is exactly as before (so long as both $CaCO_3$ and CaO are in equilibrium with CO_2).

5. What would happen in the case of $2NO(g) + Br_2(l) = 2NOBr(g)$ if we disturbed the equilibrium system by

   a. adding NOBr(g)? -- more reactants would subsequently form.
   b. adding $Br_2(l)$? -- no change (assuming the volume of the gas phase doesn't change).
   c. expanding the volume of the container? -- no change.

6. Write down the expression for the equilibrium constant for each of the following reactions:

   a. $FeO(s) + H_2(g) = Fe(s) + H_2O(g)$

   $$K = \frac{[H_2O]}{[H_2]}$$

   b. $CO_2(g) + Zn(s) = CO(g) + ZnO(s)$

   $$K = \frac{[CO]}{[CO_2]}$$

   c. $Fe_2O_3(s) + 3H_2(g) = 2Fe(s) + 3H_2O(g)$

   $$K = \frac{[H_2O]^3}{[H_2]^3}$$

Sample run of LECHAT (BASIC version)

```
DO YOU WANT AN INTRODUCTION? (YES OR NO)
?YES
THIS PROGRAM ILLUSTRATES LE CHATELIER'S PRINCIPLE BY
ALLOWING YOU TO VARY THE PARAMETERS OF A SYSTEM AT
EQUILIBRIUM,NOTING THE EFFECT.  AN INITIAL SYSTEM
IS SHOWN WITH MOLECULES A, B, AND C IN A ONE LITER
FLASK FOR THE REACTION:
          A <==> B + C
 WHERE A, B, AND C ARE GASEOUS MOLECULES.


◆◆◆
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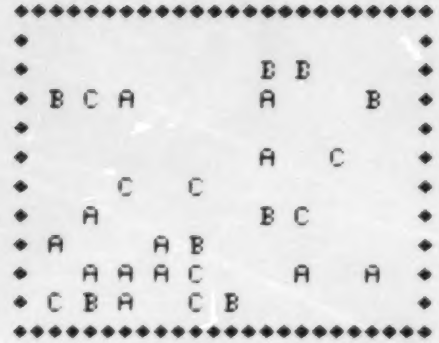

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DO YOU WANT TO TRY ANOTHER VOLUME?
?YES
CHOOSE A VOLUME BETWEEN 0.5 AND 1.5 LITERS.
?1.5
```
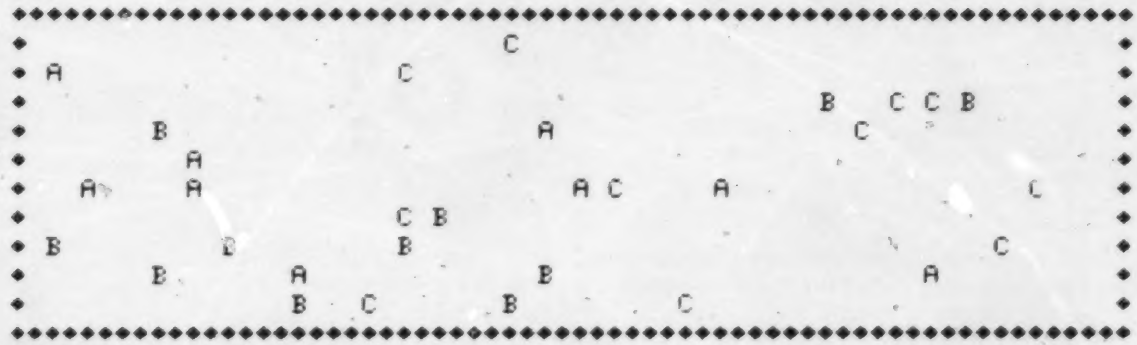
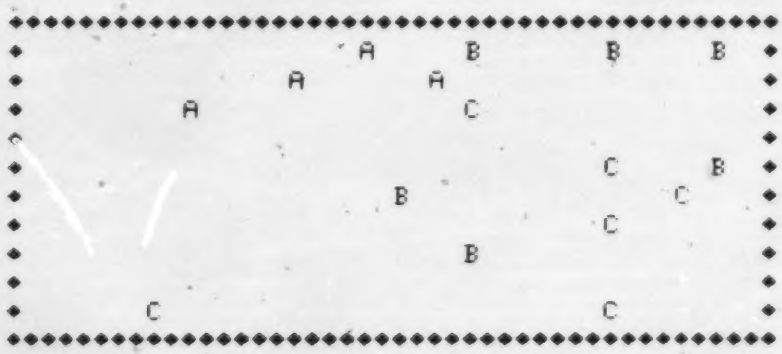
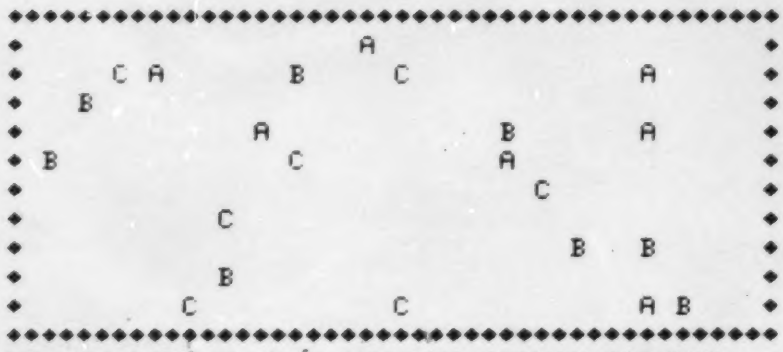



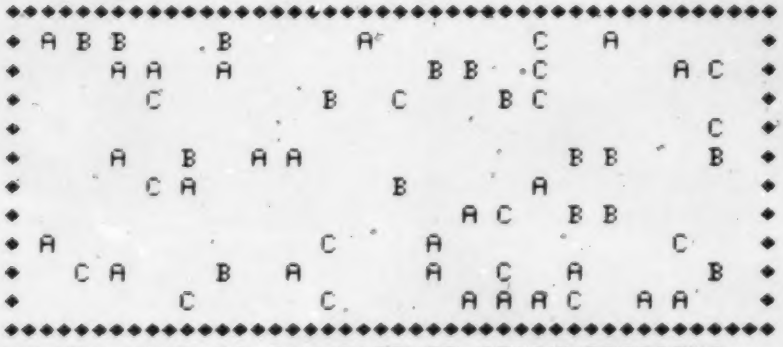
```
DO YOU WANT TO TRY ANOTHER VOLUME?
?NO
DO YOU WANT TO SEE THE EFFECT OF CHANGING THE CONCENTRATION?
?YES
CHOOSE THE INITIAL CONCENTRATIONS OF A, B, AND C
AND NOTE THE EQUILIBRIUM CONCENTRATIONS.  FOR GRAPHICAL
CONSIDERATIONS, LIMITS OF 0 TO 15 FOR THE INITIAL NUMBER
OF MOLECULES SHOULD BE USED.
?10,0,0
```



```
DO YOU WANT TO TRY ANOTHER CONCENTRATION?
?YES
CHOOSE THE INITIAL CONCENTRATIONS OF A, B, AND C
?10,5,5
```



```
DO YOU WANT TO TRY ANOTHER CONCENTRATION?
?YES
CHOOSE THE INITIAL CONCENTRATIONS OF A, B, AND C
?40,0,0
```



```
DO YOU WANT TO TRY ANOTHER CONCENTRATION?
?NO
```

LECHAT Program (in BASIC)

```
 40 REM THIS PROGRAM IS A SIMULATION OF A SYSTEM
 50 REM       A = B + C     (ALL GASES)
 60 REM WHICH IS AT EQUILIBRIUM
 70 REM USER IS ALLOWED TO VARY THE VOLUME OF THE SYSTEM
 80 REM AS WELL AS THE CONCENTRATIONS OF THE COMPONENTS
 90 REM
100 REM
110 DIM P[100,10]
120 LET K0=123
130 DEF FNR(F1)=RND(F1)
140 C9=0
150 V=20
160 L1=0
170 PRINT "DO YOU WANT AN INTRODUCTION? (YES OR NO)"
180 INPUT A$
190 IF A$<>"Y" THEN 290
200 PRINT "THIS PROGRAM ILLUSTRATES LE CHATELIER'S PRINCIPLE BY"
210 PRINT "ALLOWING YOU TO VARY THE PARAMETERS OF A SYSTEM AT"
220 PRINT "EQUILIBRIUM,NOTING THE EFFECT.  AN INITIAL SYSTEM"
230 PRINT "IS SHOWN WITH MOLECULES A, B, AND C IN A ONE LITER"
240 PRINT "FLASK FOR THE REACTION:"
250 PRINT "           A <==> B + C"
260 PRINT " WHERE A, B, AND C ARE GASEOUS MOLECULES."
270 PRINT ""
280 GOTO 340
290 PRINT "DO YOU WANT TO STUDY THE EFFECTS OF VOLUME FIRST, OR"
300 PRINT "CONCENTRATION? (TYPE V OR C)"
310 INPUT A$
320 IF A$="V" THEN 500
330 GOTO 640
340 LET V=1
350 N[1]=10
360 N[2]=10
370 N[3]=10
380 V=20*V
390 GOSUB 940
400 PRINT ""
410 GOSUB 1260
420 PRINT "DO YOU WANT TO SEE THE EFFECT OF CHANGING THE VOLUME?"
430 INPUT A$
440 IF A$="Y" THEN 500
450 PRINT &
    "DO YOU WANT TO SEE THE EFFECT OF CHANGING THE CONCENTRATION?"
460 INPUT A$
470 IF A$="Y" THEN 640
480 STOP
490 PRINT ""
500 PRINT "CHOOSE A VOLUME BETWEEN 0.5 AND 1.5 LITERS."
510 INPUT V
520 IF V<.5 THEN 500
530 IF V>1.5 THEN 500
540 LET N[2]=(-10*V+SQR(100*V**2+800*V))/2+.3
550 LET N[2]=INT(N[2])
```

```
560 N[1]=20-N[2]
570 V=20*V
580 N[3]=N[2]
590 GOSUB 940
600 PRINT ""
610 GOSUB 1260
620 PRINT "DO YOU WANT TO TRY ANOTHER VOLUME?"
630 GOTO 430
640 PRINT "CHOOSE THE INITIAL CONCENTRATIONS OF A, B, AND C"
650 IF C9<>0 THEN 700
660 PRINT "AND NOTE THE EQUILIBRIUM CONCENTRATIONS.  FOR GRAPHICAL"
670 PRINT "CONSIDERATIONS, LIMITS OF 0 TO 15 FOR THE INITIAL NUMBER"
680 PRINT "OF MOLECULES SHOULD BE USED."
690 C9=1
700 INPUT A0,B0,C0
710 T=A0+B0+C0
720 IF A0<0 THEN 780
730 IF B0<0 THEN 780
740 IF C0<0 THEN 780
750 IF T>5 THEN 800
760 PRINT "TRY LARGER CONCENTRATIONS."
770 GOTO 700
780 PRINT "USE CONCENTRATIONS WHICH ARE POSITIVE."
790 GOTO 700
800 B0=B0+A0
810 C0=C0+A0
820 A0=0
830 LET P9=((B0+C0+10)-SQR((B0+C0+10)**2-4*(B0*C0)))/2+.5
840 P9=INT(P9)
850 N[2]=B0-P9
860 N[3]=C0-P9
870 N[1]=P9
880 V=20
890 GOSUB 940
900 PRINT ""
910 GOSUB 1260
920 PRINT "DO YOU WANT TO TRY ANOTHER CONCENTRATION?"
930 GOTO 460
940 LET T=N[1]+N[2]+N[3]
950 IF T>100 THEN 1240
960 FOR I=1 TO 10
970   FOR J=1 TO 100
980     P[J,I]=0
990   NEXT J
1000 NEXT I
1010 K=1
1020 J=1
1030 I=1
1040 P[J,K]=1
1050 IF I<=N[1]+N[2] THEN P[J,K]=2
1060 IF I<=N[1] THEN P[J,K]=3
1070 I=I+1
1080 IF I>T THEN 1140
1090 K=K+1
```

```
1100 IF K<=10 THEN 1040
1110 K=1
1120 J=J+1
1130 GOTO 1040
1140 FOR I=1 TO J
1150   FOR K=1 TO 10
1160     H1=INT(V*FNR(K0)+1)
1170     V1=INT(10*FNR(K0)+1)
1180     W3=P[I,K]
1190     P[I,K]=P[H1,V1]
1200     P[H1,V1]=W3
1210   NEXT K
1220 NEXT I
1230 RETURN
1240 PRINT "YOU HAVE CHOSEN TOO MANY MOLECULES.  TRY SMALLER NUMBERS."
1250 GOTO 700
1260 V=INT(V+.49)
1270 FOR I=1 TO V
1280   PRINT "**";
1290 NEXT I
1300 PRINT "****"
1310 J=1
1320 FOR I=1 TO 10
1330   PRINT "* ";
1340   FOR I1=1 TO V
1350     IF P[I1,I]=3 THEN PRINT "A ";
1360     IF P[I1,I]=2 THEN PRINT "B ";
1370     IF P[I1,I]=1 THEN PRINT "C ";
1380     IF P[I1,I]=0 THEN PRINT "  ";
1390   NEXT I1
1400   PRINT " *"
1410 NEXT I
1420 FOR I=1 TO V
1430   PRINT "**";
1440 NEXT I
1450 PRINT "****"
1460 RETURN
1470 END
>
```